d-wave pairing in lightly doped Mott insulators

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(Dated: February 2, 2008)

We define a suitable quantity Z_c that measures the pairing strength of two electrons added to the ground state wave function by means of the anomalous part of the one-particle Green's function. Z_c discriminates between systems described by one-electron states, like ordinary metals and band insulators, for which $Z_c = 0$, and systems where the single particle picture does not hold, like superconductors and resonating valence bond insulators, for which $Z_c \neq 0$. By using a numerically exact projection technique for the Hubbard model at $U/t = 4$, a finite value of Z_c, with d-wave symmetry, is found at half filling and in the lightly doped regime, thus emphasizing a qualitatively new feature coming from electronic correlation.

Since the discovery of high-temperature (HTc) superconductors, the question whether a strongly correlated system, containing *only* repulsive interactions, may display a superconducting ground state, has been intensively debated until now, mainly because HTc superconductors are certainly strongly correlated and their critical temperature cannot be explained by a standard electron-phonon mechanism. Indeed, any mean-field approximation fails to explain superconductivity without an electron-electron attraction, that could be either explicit, like in the attractive Hubbard model, or mediated by some boson, like in the BCS theory. On the other hand, it is well known that correlated wave functions, that highly improve the mean-field energies, usually favor superconductivity. [1, 2, 3, 4, 5] Recently, the approach based on projected superconducting wave functions has been recently renewed, as it is possible to reproduce many important experimental aspects just by *assuming* that the ground state is described by a projected BCS wave function. [3, 6] Within this scheme, the superconductivity is "hidden" in the insulating state, where phase coherence is inhibited by the charge gap, and it is indeed stabilized by a small amount of doping. Unfortunately, the validity of this scenario for the actual ground state of a microscopic model remains an highly debated and controversial issue, despite a huge amount of numerical work. [5, 7, 8, 9, 10]

In this letter, we present a numerical study in favor of the mentioned scenario. We consider the single-band Hubbard model on L-site clusters:

$$H = -t \sum_{\langle i,j \rangle,\sigma} c_{i,\sigma}^\dagger c_{\sigma,j} + h.c. + U \sum_i n_{i,\uparrow} n_{i,\downarrow} - \mu N, \quad (1)$$

where $c_{i,\sigma}^\dagger$ creates an electron with spin σ at the site i, $n_{i,\sigma} = c_{i,\sigma}^\dagger c_{i,\sigma}$ is the density operator at the site i, μ is the chemical potential, and $N = \sum_{i,\sigma} n_{i,\sigma}$ is the total number of particles. We use square lattices tilted by $45°$ with $L^2 = 2l^2$ and l odd with periodic boundary conditions, so that the half-filled case ($N = L$) has a non-degenerate ground state even at $U = 0$. This condition

strongly reduces the size effects, particularly important in two dimensions (2D).

Our purpose is to study the anomalous part of the equal-time Green's function at zero temperature:

$$F_k^{BSP} = \langle \Psi_0 | c_{k,\uparrow}^\dagger c_{-k,\downarrow}^\dagger | \Psi_0 \rangle, \quad (2)$$

where $|\Psi_0\rangle$ is the ground state of the Hamiltonian H. Obviously, F_k^{BSP} can be non zero only in the thermodynamic limit, where, because of the broken symmetry phenomenon (BSP), $|\Psi_0\rangle$ may not have a definite number of particles. On a finite system BSP does not occur and F_k^{BSP} is always zero, the ground state $|\Psi_0\rangle$ having always a definite number of particles N. Therefore, on finite systems, it is useful to consider a related quantity:

$$F_k = \langle \Psi_0^{N+2} | c_{k,\uparrow}^\dagger c_{-k,\downarrow}^\dagger | \Psi_0^N \rangle, \quad (3)$$

where $|\Psi_0^N\rangle$ is the ground state with N particles. Following well known concepts of BSP, by adding to the Hamiltonian a small anomalous term, that breaks the symmetry, proportional to δ, and taking the limit $\delta \to 0$, after the thermodynamic limit, it is easy to convince that the finite-size expression F_k converges to F_k^{BSP}.

In order to evaluate F_k, we consider a trial BCS wave function $|\Psi_G\rangle$ containing only components with even number of particles:

$$|\Psi_G\rangle = \mathcal{J} \exp\left(\sum_k f_k c_{k,\uparrow}^\dagger c_{-k,\downarrow}^\dagger \right) |0\rangle, \quad (4)$$

where $|0\rangle$ is the vacuum, $f_k = \Delta_k/(\epsilon_k - \mu_0 + E_k)$, $\epsilon_k = -2t(\cos k_x + \cos k_y)$ is the free-electron dispersion, μ_0 is a variational parameter playing the role of the chemical potential of the BCS Hamiltonian, Δ_k is the corresponding gap function chosen to have either a d-wave symmetry $\Delta_k = \Delta(\cos k_x - \cos k_y)$ or an s-wave symmetry $\Delta_k = \Delta$, and $E_k = \sqrt{(\epsilon_k - \mu_0)^2 + \Delta_k^2}$. The correlation factor $\mathcal{J} = e^{-g \sum_i n_{i,\uparrow} n_{i,\downarrow}}$, g being a variational parameter, partially projects out expensive energy configurations with doubly occupied sites. In the following,

we assume that, as verified on small clusters, for an appropriate gap function symmetry, the N-particle ground state of H have non-vanishing overlap with $|\Psi_G\rangle$, at least for $N = N^*$ and $N = N^* + 2$, where $N = N^*$ represents a closed shell density. Then, on each finite system, we compute for fixed imaginary time τ:

$$F_k(\tau) = \frac{\langle \Psi_G | e^{-\tau H/2} c_{k,\uparrow}^\dagger c_{-k,\downarrow}^\dagger e^{-\tau H/2} | \Psi_G \rangle}{\langle \Psi_G | e^{-\tau H} | \Psi_G \rangle}. \qquad (5)$$

$F_k(\tau)$ will be finite even on a finite size, because the trial function $|\Psi_G\rangle$ contains sectors with different N, namely $|\Psi_G\rangle = \sum_N a_N |\Psi_G^N\rangle$. Then for large τ:

$$F_k(\tau) = F_k \frac{b_{N^*+2}}{b_{N^*}} e^{-\tau \Delta_c/2} \qquad (6)$$

where N^* is chosen by fixing the true chemical potential μ, Δ_c is the energy gap between the states with N^* and $N^* + 2$, and $b_N = \langle \Psi_G^N | \Psi_0^N \rangle a_N$. Therefore, in order to estimate F_k, the overall factor $\gamma = b_{N^*+2}/b_{N^*} e^{-\tau \Delta_c/2}$ of Eq. (6) must be computed by evaluating the average number of particles $\langle N \rangle = N^* + 2\gamma^2/(1+\gamma^2)$. An efficient choice of $|\Psi_G\rangle$ is obtained by tuning μ_0 very close to the energy level $\bar{\epsilon}_k$ with $N^* + 2$ particles, and $\Delta \ll |\bar{\epsilon}_k - \mu_0|$. In this limit, $|\Psi_G\rangle$ essentially contains only two components in the sectors with $N = N^*$ and $N = N^* + 2$ and the imaginary time projection can be done without paying much attention to the chemical potential, the number of particles being conserved by H.

The superconducting order parameter P is simply related to the short-distance component of the real-space Fourier transform $F_R = 1/L \sum_k e^{ikR} F_k$, namely $P_d = 2F_\eta$, with $\eta = (\pm 1, 0)$ or $\eta = (0, \pm 1)$ for a d-wave superconductor with $\Delta_k = \Delta(\cos k_x - \cos k_y)$, and $P_s = F_\eta$ with $\eta = (0,0)$ for an s-wave superconductor with $\Delta_k = \Delta$. Based on the resonating-valence bond (RVB) theory, [11] we want to define a quantity, closely related to F_k, that makes sense also when $P_d = 0$, as in the insulating case. Indeed, according to the RVB theory, the insulator already contains some sort of pairing, the electrons being paired in RVB singlets. Following this paradigm, we normalize the anomalous pairing function in real space and define the quantity:

$$g_R = \frac{F_R}{\sqrt{\sum_{R'} F_{R'}^2}}, \qquad (7)$$

where the sum is for all distances in the lattice (compatible with the symmetry of F_R). Notice that, also for an infinite system with a charge gap, like the half-filled Hubbard model, though the anomalous average F_R is zero, a finite ratio g_R is still possible. g_R^2 may be interpreted as the probability function of two electrons added into a singlet state at a distance R and, therefore, determines the pair function, which is the Cooper pair if $P > 0$. For a BCS superconductor with a full gap (e.g., s-wave) g_R
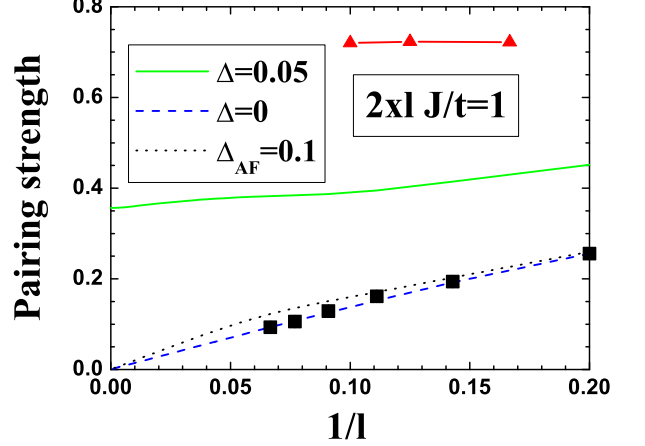

FIG. 1: Size scaling of the d-wave pairing strength Z_c for different wave functions at half-filling: the uncorrelated BCS wave function with $\Delta = 0.05$, the free-electron wave function ($\Delta \to 0$), the wave function with a finite antiferromagnetic order parameter [obtained by adding to the $\Delta \to 0$ BCS Hamiltonian a further antiferromagnetic mean field term $(-1)^i \Delta_{AF}(n_{i,\uparrow} - n_{i,\downarrow})$], and the Gutzwiller wave function with $g = 1$ (full squares). The same quantity for the exact ground state of the two-chain $t-J$ ladder at low doping is also shown (full triangles).

is localized with a well defined coherence length, whereas if the pairing function has nodes, like in the d-wave case, g_R decays with a power law, but, nonetheless, it exists a *finite* amplitude of the pairing function at short distance. In strong-coupling superconductivity, the coherence length is expected to be small, and the most important contribution to the pairing function is at the shortest distance η allowed by the symmetry of the pairing function. Therefore, we define a fundamental quantity, the *pairing strength*, that we denote by:

$$Z_c = |g_\eta|. \qquad (8)$$

As shown in Fig. 1, in the thermodynamic limit, Z_c is finite in an uncorrelated d-wave superconductor and, instead, it vanishes for free electrons, for a weakly-correlated Fermi liquid, described by a Gutzwiller wave function, and for a spin-density wave state, with a finite antiferromagnetic order parameter. By introducing the pairing strength Z_c, we provide a general and quantitative definition of pairing, which holds not only for simple superconductor systems, but also for non-BCS systems. A simple example is the two-leg ladder (see Fig. 1), where off-diagonal long-range order is suppressed by one-dimensional quantum fluctuations, but, nevertheless, Z_c remains finite, showing that pairing is well defined also in this system, as widely accepted. [12, 13, 14]

There is also another important reason to study the pairing strength Z_c instead of the order parameter P: in a strongly correlated system the value of the quasipar-
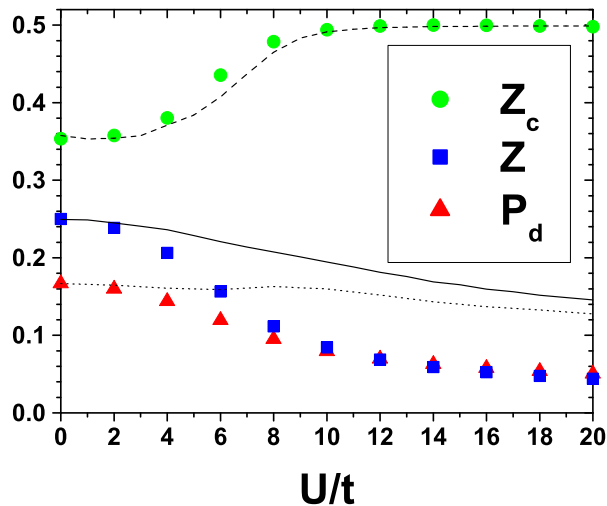
FIG. 2: The d-wave pairing strength Z_c (circles) as a function of U in an $L = 18$ site cluster with $N^* = L$. The quasiparticle weight Z_N for $N = 16$ (squares) at the momentum $(2\pi/3, 0)$ and the short-distance anomalous average P_d (triangles) are also shown. Continuous (Z_N), long dashed (Z_c) and dotted (P_d) lines correspond to the variational calculation with the variational wave function of Eq. (4) with an optimized Δ_k and projected onto the subspaces with 16 and 18 electrons.

ticle weight Z_N, defined as $Z_N = |\langle \Psi_0^{N+1}|c_k^\dagger|\Psi_0^N \rangle|^2$, can be very small [15, 16] and P, if finite, is expected to be at most of the same order. Therefore, whenever Z_N is very small, it is very difficult to detect a non-zero value of the anomalous average P. The suppression of d-wave pairing obtained in previous calculations [8, 9] can be explained by the fact that the quasiparticle weight decreases very rapidly with U (see below and Ref. [17]). The question of a finite anomalous average of order Z_N could be still compatible with the published numerical calculations and it is beyond the scope of this work. For this reason it is very difficult, at the present time, to detect pairing by studying directly the order parameter or the pairing correlations. On the other hand, the pairing strength Z_c, being a ratio of two quantities of the same order, is not affected by the small quasiparticle weight Z_N and, therefore, represents a much more sensitive detector of superconductivity. Strictly speaking, the fact of having a finite Z_c in the thermodynamic limit does not imply that also P is finite, but only the presence of paired electrons, as in the example of the two-leg ladder. However, in 2D, whenever the compressibility is finite, it is reasonable to expect condensation of pairs. Unfortunately, this assumption cannot be supported by direct calculation in the case of the Hubbard model. Nevertheless, we can safely discuss the d-wave pairing properties of the Hubbard model because a non-zero value of Z_c appears very clearly.
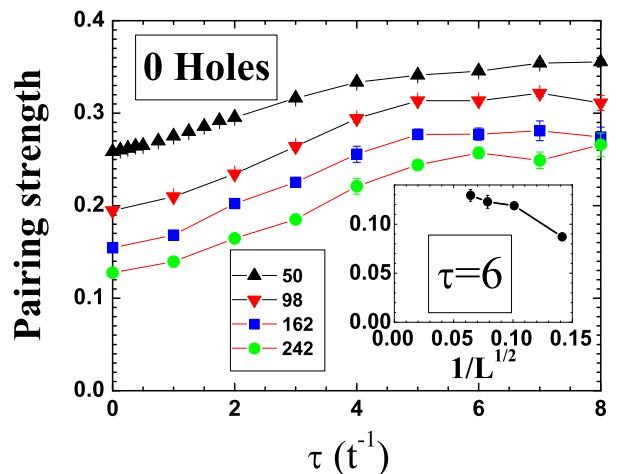
Before considering the quantum Monte Carlo results,

FIG. 3: The d-wave pairing strength Z_c as a function of the projection time τ for different clusters at half-filling. The inset shows the finite size scaling of $Z_c - Z_c^G$ for $\tau = 6$.

we show the results for a small lattice of $L = 18$ sites, where it is possible to perform exact diagonalization. In Fig. 2, we report the results for Z_c, P_d and Z_N as a function of U/t. The comparison between P_d and Z_N clearly supports our picture: P_d is small in the strong-coupling Hubbard model because Z_N is small. On the other hand, a much higher signal of paired electrons can be obtained by studying the pairing strength Z_c, which shows a broad maximum $Z_c \simeq 0.5$ for $U/t \simeq 16$, decreasing to the minimum value $Z_c \simeq 0.16$ for $U \to \infty$. Although the value of the anomalous average P_d and the quasiparticle weight are highly overestimated at strong coupling, the variational wave function of Eq. (4) with an optimized Δ_k provides an excellent estimate of Z_c for all values of $U/t \lesssim 20$, thus capturing the correct feature of pairing.

We now turn to larger systems and calculate the pairing strength by using the zero-temperature Monte Carlo projection technique based on auxiliary fields. [18] The inclusion of the simple Gutzwiller factor $\mathcal{J}$, which improves substantially the convergence in imaginary time τ, is particularly important because, at finite doping, the sign problem prevents us to work with arbitrary large imaginary time.

Firstly, we consider the half-filled case. Remarkably, for large systems, Z_c increases with the projection time τ, see Fig. 3. In this case, in order to reduce size effects, we have performed the finite-size scaling of $Z_c - Z_c^G$, where Z_c^G is the value corresponding to the Gutzwiller wave function $|\Psi_G\rangle$ with $\Delta \to 0$ ($Z_c^G \to 0$ in the thermodynamic limit, see Fig. 1). Already for $L = 50$ sites, the evaluation of the pairing strength is rather accurate and close to larger sizes. As shown in Fig. 3, Z_c increases monotonically with τ, and the value for $\tau = 6$ should safely represent, for all sizes considered, a rather accurate
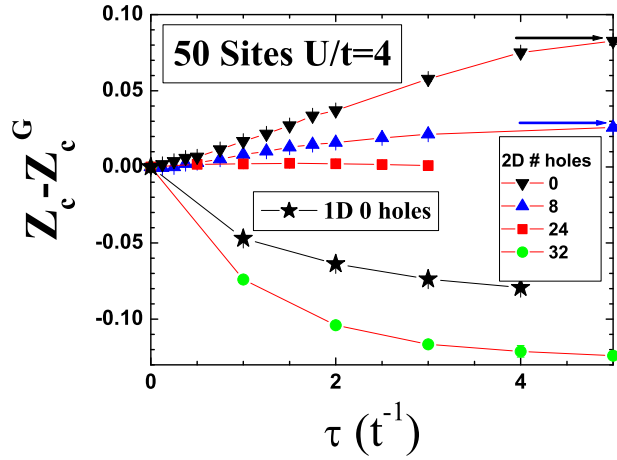
FIG. 4: The d-wave pairing strength $Z_c - Z_c^G$ as a function of the projection time τ for different dopings. The arrows indicate the value of Z_c corresponding to the variational wave function of Eq. (4) with an optimized Δ_k for 0 and 8 holes. Z_c for the s-wave pairing in one dimension is also shown.

lower bound for the $\tau \to \infty$ limit. The thermodynamic limit of Z_c appears therefore clearly finite, considering also that for $\tau = 6$ $Z_c - Z_c^G$ *increases* with the system size, see the inset of Fig. 3. Our extrapolation is consistent with a *finite* $Z_c \gtrsim 0.1$ in the thermodynamic limit. It is worth noting that, in this case, a finite value of Z_c does not mean that the ground state is superconducting, but only that two added electrons in the half-filled Hubbard model are paired together in a d-wave singlet.

In the doped case the limitation of the sign problem and the strong dependence upon hole doping prevent us to perform an accurate finite size scaling, but, as shown in Fig. 4, the effect remains rather clear, and $Z_c - Z_c^G$ increases immediately as soon as the projection time is turned on. On the other hand, at large enough doping, we have found the opposite effect, clearly against d-wave pairing. Interestingly, also the s-wave pairing strength, obtained by using an initial wave function $|\Psi_G\rangle$ with s-wave symmetry, is not enhanced by the imaginary time projection (not shown). However, we have not checked other symmetry sectors like p or d_{xy} and, therefore, at large doping there maybe other types of pairing instabilities. [19] It is remarkable that also for 50 sites the simple Gutzwiller wave function with a finite d-wave gap function (stabilized in the underdoped region) describes accurately the enhanced pairing strength Z_c, as shown by the arrows in Fig. 4.

Although we worked at zero temperature, one should be tempted to associate Z_c with the pseudogap observed in the HTc superconductors. In this scenario, the onset of the pseudogap, for a temperature T^*, is marked by a finite value of Z_c, indicating paired electrons without phase coherence, then at a much lower temperature T_c the pairs eventually condense, giving rise to a true long-range order. [20]

In conclusion, it turns out that the pairing is a robust property of lightly-doped Mott insulators and appears already in small size calculations. The pairing strength Z_c increases with decreasing doping and has its maximum at half filling, where phase coherence is inhibited by the charge gap. Notice that this is a peculiar feature of the 2D model, as in one dimension no evidence of a finite pairing strength is found even at half filling, see Fig. 4. We argue that a finite pairing strength for an insulator is just the qualitative new feature that discriminates a band insulator from a 2D RVB insulator, which is defined in terms of singlet pairs, as in a fully projected BCS wavefunction of Eq. (4). Within this definition, determined by the measurable quantity Z_c, and *independent of the variational ansatz*, we discover the possibility to have an RVB-like insulator also when the existence of a finite pairing strength is accompanied by the antiferromagnetic long-range order, like in the half-filled Hubbard model. [21] In this simple model, the insulator is somehow prepared to become superconductor (with d-wave symmetry) and a small amount of doping allows the propagation of the RVB pairs. [11] This scenario offers a simple and natural explanation of the ultimate mechanism of HTc superconductivity.

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